# **Chapter 6**

Rock, Paper, Scissors

## **Spoilers**

In this chapter, we will:

- standardize an image dataset
- train a model to predict rock, paper, scissors poses from hand images
- use dropout layers to regularize the model
- learn how to find a learning rate to train the model
- understand how the Adam optimizer uses adaptive learning rates
- capture gradients and parameters to visualize their evolution during training
- understand how momentum and Nesterov momentum work
- use schedulers to implement learning rate changes during training

## **Jupyter Notebook**

The Jupyter notebook corresponding to <u>Chapter 6</u><sup>[93]</sup> is part of the official *Deep Learning with PyTorch Step-by-Step* repository on GitHub. You can also run it directly in **Google Colab**<sup>[94]</sup>.

If you're using a *local installation*, open your terminal or Anaconda prompt and navigate to the PyTorchStepByStep folder you cloned from GitHub. Then, *activate* the pytorchbook environment and run jupyter notebook:

```
$ conda activate pytorchbook
```

(pytorchbook)\$ jupyter notebook

If you're using Jupyter's default settings, <u>this link</u> should open Chapter 6's notebook. If not, just click on Chapter 06. ipynb in your Jupyter's home page.

### **Imports**

For the sake of organization, all libraries needed throughout the code used in any

given chapter are imported at its very beginning. For this chapter, we'll need the following imports:

```
import numpy as np
from PIL import Image
from copy import deepcopy

import torch
import torch.optim as optim
import torch.nn as nn
import torch.nn.functional as F

from torch.utils.data import DataLoader, TensorDataset, random_split
from torchvision.transforms.v2 import Compose, ToImage, Normalize, \
ToPILImage, Resize, ToDtype
from torchvision.datasets import ImageFolder
from torch.optim.lr_scheduler import StepLR, ReduceLROnPlateau, \
MultiStepLR, CyclicLR, LambdaLR

from stepbystep.v2 import StepByStep
from data_generation.rps import download_rps
```

## Rock, Paper, Scissors...



...Lizard, Spock! The "extended" version of the game was displayed in the "The Lizard-Spock Expansion" episode of *The Big Bang Theory* series, and was developed by Sam Kass and Karen Bryla. To learn more about the extended version, visit Sam Kass' page<sup>[95]</sup> about the game.

Trivia aside, I guess you're probably a bit *bored* with the image dataset we've been using so far, right? Well, at least, it wasn't MNIST! But it is time to use a **different dataset**: *Rock Paper Scissors* (unfortunately, no lizard or Spock).

### **Rock Paper Scissors Dataset**



This dataset was created by Laurence Moroney (<a href="mailto:lmoroney@gmail.com">lmoroney@gmail.com</a> / <a href="mailto:laurencemoroney.com">laurencemoroney.com</a>) and can be found on his site: <a href="mailto:Rock Paper Scissors Dataset">Rock Paper Scissors Dataset</a>. [96]

The dataset is licensed as Creative Commons (CC BY 2.0). No changes were made to the dataset.

The dataset contains 2,892 images of diverse hands in the typical *rock*, *paper*, and *scissors* poses against a white background. This is a **synthetic dataset** as well since the images were generated using CGI techniques. Each image is 300x300 pixels in size and has four channels (RGBA).



RGBA stands for Red-Green-Blue-Alpha, which is the traditional RGB color model together with an alpha channel indicating how opaque each pixel is. Don't mind the alpha channel, it will be removed later.

The **training set** (2,520 images) can be downloaded <u>here</u><sup>[97]</sup> and the **test set** (372 images) can be downloaded <u>here</u>.<sup>[98]</sup> In the notebook, the datasets will be downloaded and extracted to rps and rps-test-set folders, respectively.

Here are some examples of its images, one for each pose.



Figure 6.1 - Rock, paper, scissors

There are three classes once again, so we can use what we learned in Chapter 5.

## **Data Preparation**

The data preparation step will be a bit more demanding this time since we'll be standardizing the images (for real this time—no min-max scaling anymore!). Besides, we can use the <u>ImageFolder</u> dataset now.

### **ImageFolder**

This is *not* a dataset itself, but a **generic dataset** that you can use with your own images provided that they are properly organized into sub-folders, with each sub-folder named after a class and containing the corresponding images.

The *Rock Paper Scissors* dataset **is** organized like that: Inside the **rps folder of the training set**, there are three sub-folders named after the three classes (rock, paper, and scissors).

```
rps/paper/paper01-000.png
rps/paper/paper01-001.png

rps/rock/rock01-000.png
rps/rock/rock01-001.png

rps/scissors/scissors01-000.png
rps/scissors/scissors01-001.png
```

The dataset is also **perfectly balanced**, with each sub-folder containing 840 images of its particular class.

The ImageFolder dataset requires only the root folder, which is the rps folder in our case. But it can take another four optional arguments:

- transform: You know that one already; it tells the dataset which transformations should be applied to each image, like the data augmentation transformations we've seen in previous chapters.
- target\_transform: So far, our targets have always been integers, so this argument wouldn't make sense; it starts making sense if your target is also an image (for instance, in a segmentation task).
- loader: A function that loads an image from a given path, in case you're using weird or atypical formats that cannot be handled by PIL.

• is\_valid\_file: A function that checks if a file is corrupted or not.

Let's create a dataset then:

#### **Temporary Dataset**

We're using only the transform optional argument here, and keeping transformations to a minimum. First, images are **resized to 28x28 pixels** (and automatically transformed to the RGB color model by the PIL loader, thus losing the alpha channel), and then are **converted to PyTorch tensors**. Smaller images will make our models faster to train, and more "CPU-friendly." Let's take the first image of the dataset and check its shape and corresponding label:

```
temp_dataset[0][0].shape, temp_dataset[0][1]
```

#### Output

```
(torch.Size([3, 28, 28]), 0)
```

Perfect!



"Wait, where is the standardization you promised?"

### **Standardization**

To standardize data points, we need to **learn their mean and standard deviation** first. What's the mean pixel value of our rock paper scissors images? And standard deviation? To compute these, we need to **load the data**. The good thing is, we have a (temporary) dataset with the resized images already! We're only missing a **data loader**.

#### Temporary DataLoader

```
1 temp_loader = DataLoader(temp_dataset, batch_size=16)
```

No need to bother with shuffling, as this is **not** the data loader we'll use to train the model anyway. We'll use it to compute statistics only. By the way, we need **statistics for each channel**, as required by the Normalize() transform.

So, let's build a function that takes a mini-batch (images and labels) and computes the **mean pixel value and standard deviation per channel of each image**, adding up the results for all images. Better yet, let's make it a method of our StepByStep class too.

#### StepByStep Method

```
@staticmethod
def statistics per channel(images, labels):
    # NCHW
    n_samples, n_channels, n_height, n_weight = images.size()
    # Flatten HW into a single dimension
    flatten_per_channel = images.reshape(n_samples, n_channels, -1)
    # Computes statistics of each image per channel
    # Average pixel value per channel
    # (n_samples, n_channels)
    means = flatten_per_channel.mean(axis=2)
    # Standard deviation of pixel values per channel
    # (n samples, n channels)
    stds = flatten_per_channel.std(axis=2)
    # Adds up statistics of all images in a mini-batch
    # (1, n_channels)
    sum_means = means.sum(axis=0)
    sum stds = stds.sum(axis=0)
    # Makes a tensor of shape (1, n_channels)
    # with the number of samples in the mini-batch
    n samples = torch.tensor([n samples]*n channels).float()
    # Stack the three tensors on top of one another
    # (3, n channels)
    return torch.stack([n_samples, sum_means, sum_stds], axis=0)
setattr(StepByStep, 'statistics_per_channel',
statistics_per_channel)
```

```
first_images, first_labels = next(iter(temp_loader))
StepByStep.statistics_per_channel(first_images, first_labels)
```

#### Output

Applying it to the first mini-batch of images, we get the results above: Each **column** represents a **channel**, and the rows are the **number** of data points, the **sum of mean values**, and the **sum of standard deviations**, respectively.

We can leverage the loader\_apply() method we created in the last chapter to get the sums for the whole dataset:

```
results = StepByStep.loader_apply(temp_loader,
    StepByStep.statistics_per_channel)
results
```

#### Output

So, we can compute the average mean value (that sounds weird, I know) and the average standard deviation, per channel. Better yet, let's make it a method that takes a data loader and returns an instance of the Normalize() transform, statistics and all:

```
@staticmethod
def make_normalizer(loader):
    total_samples, total_means, total_stds = \
        StepByStep.loader_apply(
            loader,
            StepByStep.statistics_per_channel
        )
        norm_mean = total_means / total_samples
        norm_std = total_stds / total_samples
        return Normalize(mean=norm_mean, std=norm_std)

setattr(StepByStep, 'make_normalizer', make_normalizer)
```



**IMPORTANT**: Always use the **training set** to **compute statistics** for standardization!

Now, we can use this method to create a transformation that **standardizes** our dataset:

Creating Normalizer Transform

```
1 normalizer = StepByStep.make_normalizer(temp_loader)
2 normalizer
```

#### Output

```
Normalize(mean=tensor([0.8502, 0.8215, 0.8116]),
std=tensor([0.2089, 0.2512, 0.2659]))
```

Remember that PyTorch converts the pixel values into the [0, 1] range. The average mean value of a pixel for the red (first) channel is 0.8502, while its average standard deviation is 0.2089.



In the next chapter, we'll use **pre-computed statistics** to standardize the inputs when using a **pre-trained model**.

#### The Real Datasets

It's time to build our *real* datasets using the Normalize() transform with the statistics we learned from the (temporary) training set. The data preparation step looks like this:

#### Data Preparation

```
1 composer = Compose([Resize(28),
2
                       ToImage(),
3
                       ToDtype(torch.float32, scale=True),
4
                       normalizer])
 6 train data = ImageFolder(root='rps', transform=composer)
7 val_data = ImageFolder(root='rps-test-set', transform=composer)
8
9 # Builds a loader of each set
10 train_loader = DataLoader(
       train_data, batch_size=16, shuffle=True
11
12 )
13 val_loader = DataLoader(val_data, batch_size=16)
```

Even though the second part of the dataset was named rps-test-set by its author, we'll be using it as our validation dataset. Since **each dataset**, both training and validation, corresponds to a **different folder**, there is no need to split anything.

Next, we use both datasets to create the corresponding data loaders, remembering to **shuffle the training set**.

Let's take a peek at some images from the *real* training set.

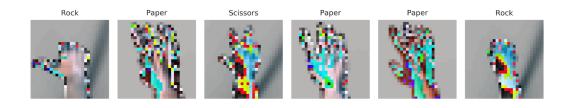


Figure 6.2 - Training set (normalized)



There is nothing wrong with the colors, it is just the **effect of the standardization of the pixel values**. Now that we have colored images, we can take a step back into the convolution world and see how it handles...

## **Three-Channel Convolutions**

Before, there was a single-channel image and a single-channel filter. Or many filters, but each of them still having a single channel. Now, there is a **three-channel image** and a **three-channel filter**. Or many filters, but each of them still having three channels.



Every **filter** has as many **channels** as the **image** it is convolving.

Convolving a three-channel filter over a three-channel image **still produces a single value**, as depicted in the figure below.

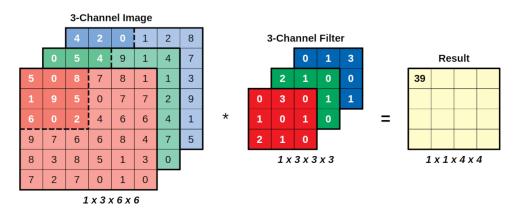


Figure 6.3 - Convolution with multiple channels

We can think of it as performing three convolutions, each corresponding to the element-wise multiplication of the matching region / channel and filter / channel, resulting in three values, one for each channel. Adding up the results for each channel produces the expected single value. The figure below should illustrate it better.

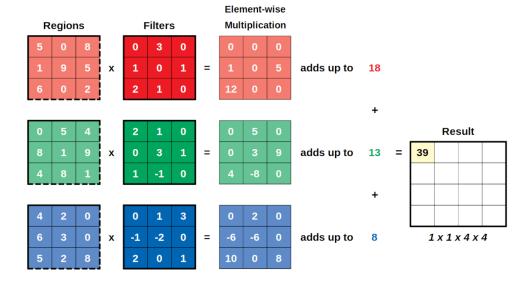


Figure 6.4 - Convolution over each channel

We can also look at it in code if you prefer:

#### Output

```
(1, 3, 3, 3)
```

#### Output

```
(1, 3, 3, 3)
```

#### Output

```
(tensor([[[[39]]]]), torch.Size([1, 1, 1, 1]))
```



"What if I have **two filters**?"

Glad you asked! The figure below illustrates the fact that **every filter** has **as many channels** as the image being convolved.

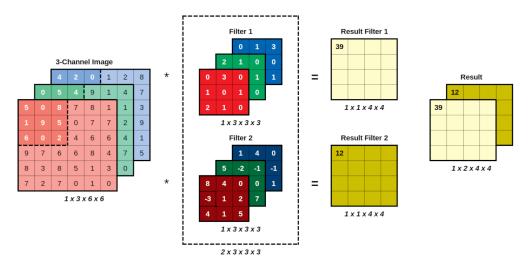


Figure 6.5 - Two filters over three channels

If you have **two filters**, and the input **image has three channels**, each **filter has three channels** as well, and the **output has two channels**.



The convolution produces as many **channels** as there are **filters**.

OK, it is time to develop a...

## **Fancier Model**

Let's leave the Sequential model aside for now and build a model class again. This time, our constructor method will take two arguments: n\_filters and p. We'll use n\_filters as the number of output channels for both convolutional blocks of our model (yes, there are two now!). And, as you can see from the code below, we'll use p as the probability of dropout.



"Dropout? What is that?"



Hold on tight, we'll get to it in the next section.

```
class CNN2(nn.Module):
    def __init__(self, n_filters, p=0.0):
        super(CNN2, self).__init__()
        self.n filters = n filters
        self.p = p
        # Creates the convolution layers
        self.conv1 = nn.Conv2d(
            in channels=3,
            out_channels=n_filters,
            kernel size=3
        )
        self.conv2 = nn.Conv2d(
            in channels=n filters,
            out_channels=n_filters,
            kernel size=3
        )
        # Creates the linear layers
        # Where does this 5 * 5 come from?! Check it below
        self.fc1 = nn.Linear(n filters * 5 * 5, 50)
        self.fc2 = nn.Linear(50, 3)
        # Creates dropout layers
        self.drop = nn.Dropout(self.p)
```

There are two convolutional layers, and two linear layers, fc1 (the hidden layer) and fc2 (the output layer).



"Where are the layers for activation functions and max pooling?"

Well, the max pooling layer **doesn't learn anything**, so we can use its **functional form**: F.max\_pool2d(). The same goes for the chosen activation function: F.relu().



If you choose the parametric ReLU (PReLU), you shouldn't use the functional form since it needs to learn the coefficient of leakage (the slope of the negative part).

On the one hand, you keep the model's attributes to a minimum. On the other hand, you don't have layers to *hook* anymore, so you **cannot capture** the output of **activation functions** and **max pooling operations** anymore.

Let's create our two convolutional blocks in a method aptly named **featurizer**:

Fancier Model (Featurizer)

```
def featurizer(self, x):
    # First convolutional block
    # 3@28x28 -> n_filters@26x26 -> n_filters@13x13
    x = self.conv1(x)
    x = F.relu(x)
    x = F.max_pool2d(x, kernel_size=2)
    # Second convolutional block
    # n_filters@13x13 -> n_filters@11x11 -> n_filters@5x5
    x = self.conv2(x)
    x = F.relu(x)
    x = F.max_pool2d(x, kernel_size=2)
    # Input dimension (n_filters@5x5)
    # Output dimension (n_filters * 5 * 5)
    x = nn.Flatten()(x)
    return x
```

This structure, where an argument x is both **input** and **output** of every operation in a sequence, is fairly common. The featurizer produces a feature tensor of size n\_filters times 25.

The next step is to build the *classifier* using the linear layers, one as a hidden layer, the other as the output layer. But there is **more** to it: There is a **dropout layer** before each linear layer, and it will **drop values with a probability p** (the second argument of our constructor method):

```
def classifier(self, x):
    # Classifier
    # Hidden Layer
    # Input dimension (n feature * 5 * 5)
    # Output dimension (50)
    if self.p > 0:
        x = self.drop(x)
    x = self.fc1(x)
    x = F.relu(x)
    # Output Layer
    # Input dimension (50)
    # Output dimension (3)
    if self.p > 0:
        x = self.drop(x)
    x = self.fc2(x)
    return x
```



"How does dropout work?"

We'll dive deeper into it in the next section, but we need to *finish* our model class first. What's left to be done? The implementation of the forward() method:

Fancier Model (Forward)

```
def forward(self, x):
    x = self.featurizer(x)
    x = self.classifier(x)
    return x
```

It takes the **inputs** (a mini-batch of images, in this case), runs them through the **featurizer** first, and then runs the produced features through the **classifier**, which produces **three logits**, one for each class.

## **Dropout**

Dropout is an important piece of deep learning models. It is used as a **regularizer**; that is, it tries to **prevent overfitting** by **forcing the model** to find **more than one way to achieve the target**.

The general idea behind **regularization** is that, if left unchecked, a model will try to find the "easy way out" (can you blame it?!) to achieve the target. What does it mean? It means it may end up **relying on a handful of features** because these features were found to be more relevant in the training set. Maybe they are, maybe they aren't—it could very well be a **statistical fluke**, who knows, right?

To make the model more robust, some of the features are randomly **denied to it**, so it has to achieve the target **in a different way**. It makes training harder, but it should result in **better generalization**; that is, the model should perform better when handling **unseen data** (like the data points in the validation set).

The whole thing looks a lot like the **randomization of features** used in **random forests** to perform the splits. Each tree, or even better, each split has access to a **subset of features only**.



"How does this, "feature randomization", work in a deep learning model?"

To illustrate it, let's build a sequential model with a single nn.Dropout layer:

```
dropping_model = nn.Sequential(nn.Dropout(p=0.5))
```



"Why do I need a model for **this**? Can't I use the **functional** form F.dropout() instead?"

Yes, a functional dropout would go just fine here, but I wanted to illustrate another point too, so please bear with me. Let's also create some neatly spaced points to make it easier to understand the effect of dropout.

```
spaced_points = torch.linspace(.1, 1.1, 11)
spaced_points
```

#### Output

```
tensor([0.1000, 0.2000, 0.3000, 0.4000, 0.5000, 0.6000, 0.7000, 0.8000, 0.9000, 1.0000, 1.1000])
```

Next, let's use these points as inputs of our amazingly simple model:

```
torch.manual_seed(44)

dropping_model.train()
output_train = dropping_model(spaced_points)
output_train
```

#### Output

```
tensor([0.0000, 0.4000, 0.0000, 0.8000, 0.0000, 1.2000, 1.4000, 1.6000, 1.8000, 0.0000, 2.2000])
```

#### There are **many things** to notice here:

- The model is in train mode (very important, hold on to this!).
- Since this model does not have any weights, it becomes clear that dropout drops inputs, not weights.
- It dropped four elements only!
- The remaining elements have different values now!



"What's going on here?"

First, dropping is probabilistic, so each input had a 50% chance of being dropped. In our tiny example, by chance, only four out of ten were actually dropped (hold on to this thought too!).

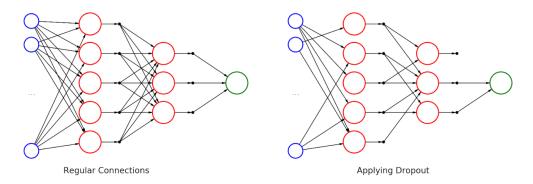


Figure 6.6 - Applying dropout

Second, the **remaining elements** need to be **proportionally adjusted by a factor of** 1/p. In our example, that's a factor of two.

```
output_train / spaced_points
```

Output

```
tensor([0., 2., 0., 2., 0., 2., 2., 2., 2., 0., 2.])
```



"Why?"

This adjustment has the purpose of **preserving** (or at least trying to) the **overall level of the outputs** in the particular layer that's "suffering" the dropout. So, let's imagine that these inputs (after dropping) will feed a **linear layer** and, for educational purposes, that all their **weights are equal to one** (and bias equals zero). As you already know, a linear layer will multiply these weights by the (dropped) inputs and sum them up:

```
F.linear(output_train, weight=torch.ones(11), bias=torch.tensor(0))
```

Output

```
tensor(9.4000)
```

The sum is 9.4. It would have been half of this (4.7) without the adjusting factor.



"OK, so what? Why do I need to preserve the level of the outputs anyway?"

Because **there** is no dropping in evaluation mode! We've talked about it briefly in the past—the dropout is **random** in nature, so it would produce slightly (or maybe not so slightly) **different predictions** for the **same inputs**. You don't want that, that's bad business. So, let's **set our model to eval mode** (and that's why I chose to make it a model instead of using functional dropout) and see what happens there:

```
dropping_model.eval()
output_eval = dropping_model(spaced_points)
output_eval
```

```
tensor([0.1000, 0.2000, 0.3000, 0.4000, 0.5000, 0.6000, 0.7000, 0.8000, 0.9000, 1.0000, 1.1000])
```

Pretty boring, right? This isn't doing anything!



Finally, an **actual difference in behavior** between train and eval modes! It was long overdue!

The inputs are just **passing through**. What's the implication of this? Well, that **linear layer** that receives these values is still multiplying them by the weights and summing them up:

```
F.linear(output_eval, weight=torch.ones(11), bias=torch.tensor(\emptyset))
```

Output

```
tensor(6.6000)
```

This is the sum of **all inputs** (because all the weights were set to one and no input was dropped). If there was no adjusting factor, the outputs in evaluation and training modes would be substantially different, simply because there would be **more terms to add up** in **evaluation mode**.



"I am still not convinced ... without adjusting the output would be 4.7, which is closer to 6.6 than the adjusted 9.4 ... what is up?"

This happened because dropping is **probabilistic**, and only four out of ten elements were actually dropped (that was the thought I asked you to hold on to). The factor **adjusts for the average number of dropped elements**. We set the probability to 50% so, **on average, five elements will be dropped**. By the way, if you change the seed to 45 and re-run the code, it will *actually* drop half of the inputs, and the adjusted output will be 6.4 instead of 9.4.

Instead of setting a different random seed and manually checking which value it produces, let's generate 1,000 scenarios and compute the **sum of the adjusted dropped outputs** to get their distribution:

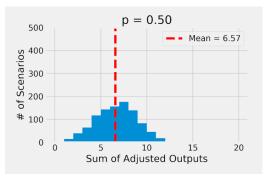


Figure 6.7 - Distribution of outputs

The figure above shows us that, for that set of inputs, the output of our simple linear layer with dropout will **not be exactly 6.6** anymore, but **something between 0 and 12**. The mean value for all scenarios is *quite close* to 6.6, though.

Dropout not only **drops some inputs** but, due to its probabilistic nature, **produces a distribution of outputs**.



In other words, the model needs to learn how to handle a distribution of values that is centered at the value the output would have if there was no dropout.

Moreover, the choice of the **dropout probability** determines **how spread out** the outputs will be.

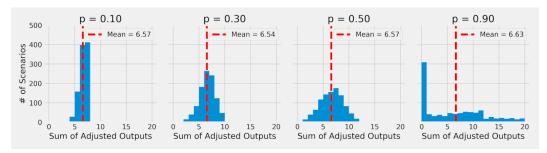


Figure 6.8 - Output distribution for dropout probabilities

On the left, if there is barely any dropout (p=0.10), the sum of adjusted outputs is tightly distributed around the mean value. For more **typical dropout probabilities** (like 30% or 50%), the distribution **may** take some more extreme values.

If we go to **extremes**, like a dropout probability of 90%, the distribution gets a *bit* degenerated, I would say—it is pretty much all over the place (and it has a lot of scenarios where *everything gets dropped*, hence the tall bar at zero).



The variance of the distribution of outputs grows with the dropout probability.

A higher dropout probability makes it harder for your model to learn—that's what regularization does.



"Can I use **dropout** with the **convolutional layers**?"

## **Two-Dimensional Dropout**

Yes, you can, but not that dropout. There is a specific dropout to be used with convolutional layers: nn.Dropout2d. Its dropout procedure is a bit different, though: Instead of dropping individual inputs (which would be pixel values in a given channel), it drops entire channels / filters. So, if a convolutional layer produces ten filters, a two-dimensional dropout with a probability of 50% would drop five filters (on average), while the remaining filters would have all their pixel values left untouched.



"Why does it drop entire channels instead of dropping pixels?"

Randomly dropping pixels doesn't do much for regularization because **adjacent pixels are strongly correlated**; that is, they have quite similar values. You can think of it this way: If there are some **dead pixels randomly spread in an image**, the

missing pixels can probably be easily filled with the values of the adjacent pixels. On the other hand, if a full channel is dropped (in an RGB image), the **color changes** (good luck figuring out the values for the missing channel!).

The figure below illustrates the effect of both regular and two-dimensional dropout procedures on an image of our dataset.



Figure 6.9 - Dropping channels with nn. Dropout 2d

Sure, in deeper layers, there is no correspondence between channel and color anymore, but each channel still encodes *some feature*. By randomly dropping some channels, two-dimensional dropout achieves the desired regularization.

Now, let's make it *a bit harder* for our model to learn by setting its dropout probability to 30% and observing how it fares...

## **Model Configuration**

The configuration part is short and straightforward: We create a **model**, a **loss function**, and an **optimizer**.

The model will be an instance of our CNN2 class with **five filters** and a **dropout probability of 30%**. Our dataset has three classes, so we're using nn.CrossEntropyLoss() (which will take the **three logits** produced by our model).

### **Optimizer**

Regarding the **optimizer**, let's *ditch* the SGD optimizer and use *Adam* for a change. Stochastic gradient descent is *simple and straightforward*, as we've learned in Chapter 0, but it is also *slow*. So far, the training speed of SGD has not been an issue because our problems were quite simple. But, as our models grow a bit more complex, we can benefit from choosing a different optimizer.

Adaptive moment estimation (Adam) uses adaptive learning rates, computing a learning rate for each parameter. Yes, you read it right: Each parameter has a learning rate to call its own!



If you dig into the state\_dict() of an Adam optimizer, you'll find tensors shaped like the parameters of every layer in your model that Adam will use to compute the corresponding learning rates. True story!

<u>Adam</u> is known to achieve good results **fast** and is likely a safe choice of optimizer. We'll get back to its inner workings in a later section.

### **Learning Rate**

Another thing we need to keep in mind is that 0.1 won't cut it as a learning rate anymore. Remember what happens when the learning rate is **too high**? The loss doesn't go down or, even worse, goes up! We need to go **lower**, **much lower**, than that. For this example, let's use **3e-4**, the <u>"Karpathy's Constant." [99]</u> Even though it was meant as a joke, it still is in the right order of magnitude, so let's give it a try.

#### Model Configuration

```
1 torch.manual_seed(13)
2 model_cnn2 = CNN2(n_feature=5, p=0.3)
3 multi_loss_fn = nn.CrossEntropyLoss(reduction='mean')
4 optimizer_cnn2 = optim.Adam(model_cnn2.parameters(), lr=3e-4)
```

We have everything in place to start the...

## **Model Training**

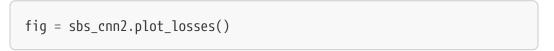
Once again, we use our StepByStep class to handle model training for us.

#### **Model Training**

```
1 sbs_cnn2 = StepByStep(model_cnn2, multi_loss_fn, optimizer_cnn2)
2 sbs_cnn2.set_loaders(train_loader, val_loader)
3 sbs_cnn2.train(10)
```

You should expect training to take a while since this model is more complex than

previous ones (6,823 parameters against 213 parameters for the last chapter's model). After it finishes, the computed losses should look like this:



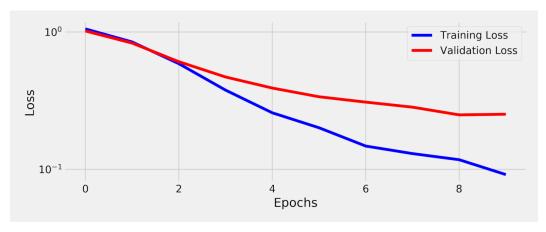


Figure 6.10 - Losses

### **Accuracy**

We can also check the model's accuracy for each class:

```
StepByStep.loader_apply(val_loader, sbs_cnn2.correct)
```

#### Output

The model got 313 out of 372 right. That's 84.1% accuracy on the validation set—not bad!

### **Regularizing Effect**

Dropout layers are used for **regularizing**; that is, they should **reduce overfitting** and **improve generalization**. Or so they say :-)

Let's (empirically) verify this claim by training a model identical in every way BUT the dropout, and compare its losses and accuracy to the original model.

Then, we can plot the losses of the model above (*no dropout*) together with the losses from our previous model (30% dropout):

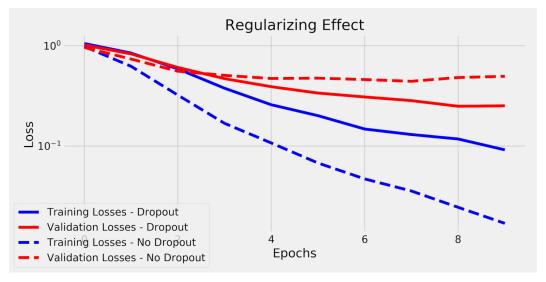


Figure 6.11 - Losses (with and without regularization)

This is actually a very nice depiction of the regularizing effect of using dropout:

- Training loss is **higher** with **dropout**—after all, dropout makes training harder.
- Validation loss is lower with dropout—it means that the model is generalizing better and achieving a better performance on unseen data, which is the whole point of using a regularization method like dropout.

We can also observe this effect by looking at the accuracy for both sets and

models. First, the **no dropout** model, which is expected to **overfit to the training** data:

#### Output

```
tensor([2518, 2520]) tensor([293, 372])
```

That's 99.92% accuracy on the training set! And 78.76% on the validation set—it smells like overfitting!

Then, let's look at the regularized version of the model:

#### Output

```
tensor([2504, 2520]) tensor([313, 372])
```

That's 99.36% accuracy on the training set—still quite high! But we got 84.13% on the validation set now—a **narrower gap** between training and validation accuracy is always a good sign. You can also try **different probabilities** of dropout and observe how much better (or worse!) the results get.

## **Visualizing Filters**

There are **two** convolutional layers in this model, so let's visualize them! For the first one, **conv1**, we get:

```
model_cnn2.conv1.weight.shape
```

```
torch.Size([5, 3, 3, 3])
```

Its shape indicates it produced **five filters** for each one of the **three input channels** (15 filters in total), and each filter is 3x3 pixels.

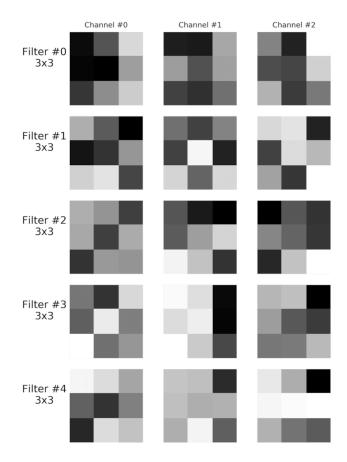


Figure 6.12 - Visualizing filters for conv1 layer

For the second convolutional layer, conv2, we get:

model\_cnn2.conv2.weight.shape

```
torch.Size([5, 5, 3, 3])
```

Its shape indicates it produced **five filters** for each one of the **five input channels** (25 filters in total), and each filter is 3x3 pixels.

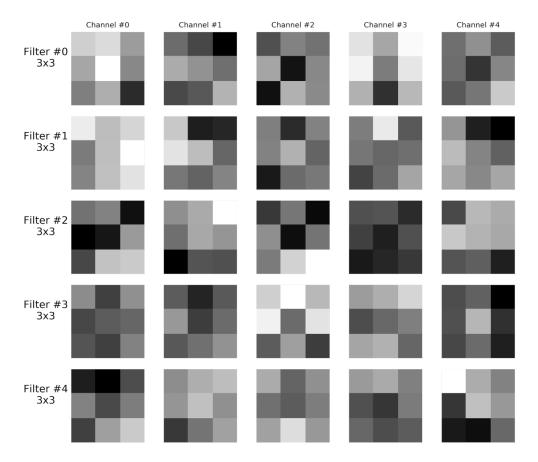


Figure 6.13 - Visualizing filters for conv2 layer

## **Learning Rates**

It is time to have "the talk." It cannot be postponed any longer—we need to talk about choosing a learning rate! It is no secret that the learning rate is the most important hyper-parameter of all—it drives the update of the parameters; that is, it drives how fast a model learns (hence, learning rate).

Choosing a learning rate that works well for a given model (and dataset) is a difficult task, one mostly done by **trial-and-error** since there is no analytical way of finding the *optimal* learning rate. One thing we can say for sure is that it should be **less than 1.0**, and it is likely **higher than 1e-6**.



"Well, that doesn't help much..."

Indeed, it doesn't. So, let's discuss how we can make it a bit more specific.

In previous chapters, we used **0.1** as the learning rate, which is **kind of high** but worked well for really simple problems. As models grow more complex, though, that value is definitely *too high*, and **one order of magnitude lower (0.01)** is a better **starting point**.



"What if it is still too high and the loss doesn't go down?"

That's a real possibility, and one possible way of handling this is to perform a **grid search**, trying **multiple learning rates** over a few epochs each and comparing the evolution of the losses. This is expensive, computationally speaking, since you need to train the model multiple times, but it may still be feasible if your model is not *too* large.



"How do I choose values for the grid search?"

It is common to reduce the learning rate by a **factor of 3** or a **factor of 10**. So, your learning rate values could very well be [0.1, 0.03, 0.01, 3e-3, 1e-3, 3e-4, 1e-4] (using a factor of 3) or [0.1, 0.01, 1e-3, 1e-4, 1e-5] (using a factor of 10). In general, if you plot the learning rates against their corresponding losses, this is what you can expect:

- If the learning rate is **too low**, the model doesn't learn much, and the **loss** remains high.
- If the learning rate is **too high**, the model doesn't converge to a solution, and the **loss gets higher**.
- In between those two extremes, the loss should be lower, hinting at the right order of magnitude for the learning rate.

### **Finding LR**

As it turns out, you **don't have to grid search** the learning rate like that. In 2017, Leslie N. Smith published "Cyclical Learning Rates for Training Neural Networks" in which he outlines a procedure to **quickly find an appropriate range for the initial learning rate** (more on the *cyclical* part of his paper later!). This technique is called **LR Range Test**, and it is quite a simple solution to help you get a first estimate for the appropriate learning rate.

The general idea is pretty much the same as the grid search: It tries multiple learning rates and logs the corresponding losses. But here comes the difference: It evaluates the loss over a single mini-batch, and then changes the learning rate before moving on to the next mini-batch.

This is **computationally cheap** (it is performing ONE training step only for each candidate) and can be performed **inside the same training loop**.



"Wait a minute! Wouldn't the results be affected by the previous training steps performed using different learning rates?"

Well, technically, yes. But this is not such a big deal: First, we're looking for a **ballpark estimate** of the learning rate, not a precise value; second, these updates will barely nudge the model from its initial state. It is easier to live with this difference than to reset the model every single time.

First, we need to define the **boundaries** for the test (start\_lr and end\_lr) and the **number of iterations** (num\_iter) to move from one to the other. On top of that, we can choose to change **how** to make the increments: linearly or exponentially. Let's build a higher-order function that takes all those arguments and returns another function, one that returns the multiplying factor given the current iteration number:

```
1 def make_lr_fn(start_lr, end_lr, num_iter, step_mode='exp'):
2
       if step_mode == 'linear':
           factor = (end_lr / start_lr - 1) / num_iter
3
           def lr fn(iteration):
4
               return 1 + iteration * factor
5
6
      else:
7
           factor = (np.log(end_lr) - np.log(start_lr)) / num_iter
8
           def lr fn(iteration):
9
               return np.exp(factor)**iteration
       return lr fn
10
```

Now, let's try it out: Say we'd like to try **ten different learning rates** between 0.01 and 0.1, and the increments should be exponential:

```
start_lr = 0.01
end_lr = 0.1
num_iter = 10
lr_fn = make_lr_fn(start_lr, end_lr, num_iter, step_mode='exp')
```

There is a **factor of 10** between the two rates. If we apply this function to a sequence of iteration numbers, from 0 to 10, that's what we get:

```
lr_fn(np.arange(num_iter + 1))
```

#### Output

If we **multiply** these values by the **initial learning rate**, we'll get an array of learning rates ranging from 0.01 to 0.1 as expected:

```
start_lr * lr_fn(np.arange(num_iter + 1))
```

```
array([0.01 , 0.01258925, 0.01584893, 0.01995262, 0.02511886, 0.03162278, 0.03981072, 0.05011872, 0.06309573, 0.07943282, 0.1 ])
```



"Cool, but how do I change the learning rate of an optimizer?"

Glad you asked! It turns out, we can assign a **scheduler** to an optimizer, such that it **updates the learning rate** as it goes. We're going to dive deeper into learning rate schedulers in a couple of sections. For now, it suffices to know that we can **make it follow a sequence of values like the one above** using a scheduler that takes a **custom function**. Coincidence? I think not! That's what we'll be using lr\_fn() for:

```
dummy_model = CNN2(n_feature=5, p=0.3)
dummy_optimizer = optim.Adam(dummy_model.parameters(), lr=start_lr)
dummy_scheduler = LambdaLR(dummy_optimizer, lr_lambda=lr_fn)
```

The LambdaLR scheduler takes an optimizer and a custom function as arguments and modifies the learning rate of that optimizer accordingly. To make it happen, though, we need to call the scheduler's step() method, but only after calling the optimizer's own step() method:

```
dummy_optimizer.step()
dummy_scheduler.step()
```

After **one step**, the learning rate should have been updated to match the second value in our array (0.01258925). Let's double-check it using the scheduler's **get\_last\_lr()** method:

```
dummy_scheduler.get_last_lr()[0]
```

#### Output

```
0.012589254117941673
```

Perfect! Now let's build the actual range test. This is what we're going to do:

- Since we'll be updating both **model** and **optimizer**, we need to **store their initial states** so they can be restored in the end.
- Create both **custom function** and corresponding **scheduler**, just like in the snippets above.
- (Re)implement a **training loop** over **mini-batches**, so we can **log** the **learning rate** and **loss** at every step.
- Restore model and optimizer states.

Moreover, since we're using a **single mini-batch** to evaluate the loss, the resulting values will likely jump up and down a lot. So, it is better to **smooth the curve** using an **exponentially weighted moving average (EWMA)** (we'll talk about EWMAs in much more detail in the next section) to more easily identify the trend in the values.

This is what the method looks like:

#### StepByStep Method

```
def lr range test(self, data loader, end lr, num iter=100,
                  step_mode='exp', alpha=0.05, ax=None):
    # The test updates both model and optimizer, so we need to
    # store their initial states to restore them in the end
    previous_states = {
        'model': deepcopy(self.model.state dict()),
        'optimizer': deepcopy(self.optimizer.state_dict())
    # Retrieves the learning rate set in the optimizer
    start_lr = self.optimizer.state_dict()['param_groups'][0]['lr']
    # Builds a custom function and corresponding scheduler
    lr_fn = make_lr_fn(start_lr, end_lr, num_iter)
    scheduler = LambdaLR(self.optimizer, lr_lambda=lr_fn)
    # Variables for tracking results and iterations
    tracking = {'loss': [], 'lr': []}
    iteration = 0
    # If there are more iterations than mini-batches in the data
    # loader, it will have to loop over it more than once
    while (iteration < num_iter):</pre>
```

```
# That's the typical mini-batch inner loop
    for x_batch, y_batch in data_loader:
        x batch = x batch.to(self.device)
        y_batch = y_batch.to(self.device)
        # Step 1
        yhat = self.model(x batch)
        # Step 2
        loss = self.loss_fn(yhat, y_batch)
        # Step 3
        loss.backward()
        # Here we keep track of the losses (smoothed)
        # and the learning rates
        tracking['lr'].append(scheduler.get last lr()[0])
        if iteration == 0:
            tracking['loss'].append(loss.item())
        else:
            prev_loss = tracking['loss'][-1]
            smoothed_loss = (alpha * loss.item() +
                            (1-alpha) * prev_loss)
            tracking['loss'].append(smoothed_loss)
        iteration += 1
        # Number of iterations reached
        if iteration == num_iter:
            break
        # Step 4
        self.optimizer.step()
        scheduler.step()
        self.optimizer.zero_grad()
# Restores the original states
self.optimizer.load_state_dict(previous_states['optimizer'])
self.model.load state dict(previous states['model'])
if ax is None:
    fig, ax = plt.subplots(1, 1, figsize=(6, 4))
else:
    fig = ax.get_figure()
ax.plot(tracking['lr'], tracking['loss'])
if step_mode == 'exp':
    ax.set_xscale('log')
```

```
ax.set_xlabel('Learning Rate')
ax.set_ylabel('Loss')
fig.tight_layout()
return tracking, fig

setattr(StepByStep, 'lr_range_test', lr_range_test)
```

Since the technique is supposed to be applied on an **untrained model**, we create a new model (and optimizer) here:

#### Model Configuration

```
1 torch.manual_seed(13)
2 new_model = CNN2(n_feature=5, p=0.3)
3 multi_loss_fn = nn.CrossEntropyLoss(reduction='mean')
4 new_optimizer = optim.Adam(new_model.parameters(), lr=3e-4)
```

Next, we create an instance of StepByStep and call the new method using the **training data loader**, the **upper range** for the learning rate (end\_lr), and how many iterations we'd like it to try:

#### Learning Rate Range Test

```
1 sbs_new = StepByStep(new_model, multi_loss_fn, new_optimizer)
2 tracking, fig = sbs_new.lr_range_test(
3 train_loader, end_lr=1e-1, num_iter=100)
```

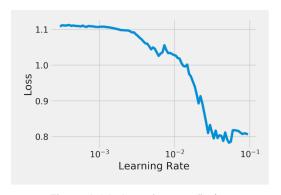


Figure 6.14 - Learning rate finder

There we go: a "U"-shaped curve. Apparently, the *Karpathy Constant* (3e-4) is **too low** for our model. The **descending part** of the curve is the region we should aim for: something around 0.01.

This means we could have used a higher learning rate, like 0.005, to train our model. But this also means we need to **recreate the optimizer** and **update it in sbs\_new**. First, let's create a method for setting its optimizer:

StepByStep Method

```
def set_optimizer(self, optimizer):
    self.optimizer = optimizer
setattr(StepByStep, 'set_optimizer', set_optimizer)
```

Then, we create and set the new optimizer and train the model as usual:

Updating LR and Model Training

```
1 new_optimizer = optim.Adam(new_model.parameters(), lr=0.005)
2 sbs_new.set_optimizer(new_optimizer)
3 sbs_new.set_loaders(train_loader, val_loader)
4 sbs_new.train(10)
```

If you try it out, you'll find that the training loss actually goes down a bit faster (and that the model might be overfitting).



**DISCLAIMER**: The learning rate finder is surely not magic! Sometimes you'll **not** get the "U"-shaped curve: Maybe the initial learning rate (as defined in your optimizer) is too high already, or maybe the end\_lr is too low. Even if you do, it does not necessarily mean the mid-point of the descending part will give you the fastest learning rate for your model.



"OK, if I manage to choose a good learning rate from the start, am I done with it?"

Sorry, but **NO**! Well, it depends; it might be fine for simpler (but real, not toy) problems. The issue here is, for larger models, the **loss surface** (remember that, from Chapter 0?) becomes **very messy**, and a **learning rate that works well at the start** of model training **may be too high for a later stage** of model training. It means that the learning rate needs to **change** or **adapt**.

## **LRFinder**

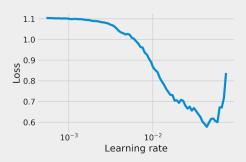
The function we've implemented above is fairly basic. For an implementation with more bells and whistles, check this Python package: <u>torch lr finder</u>. [101] I am illustrating its usage here, which is quite similar to what we've done above, but please refer to the documentation for more details.

```
!pip install --quiet torch-lr-finder
from torch_lr_finder import LRFinder
```

Instead of calling a function directly, we need to create an instance of LRFinder first, using the typical model configuration objects (model, optimizer, loss function, and the device). Then, we can take the range\_test() method for a spin, providing familiar arguments to it: a data loader, the upper range for the learning rate, and the number of iterations. The reset() method restores the original states of both model and optimizer.

```
torch.manual_seed(11)
new_model = CNN2(n_feature=5, p=0.3)
multi_loss_fn = nn.CrossEntropyLoss(reduction='mean')
new_optimizer = optim.Adam(new_model.parameters(), lr=3e-4)
device = 'cuda' if torch.cuda.is_available() else 'cpu'

lr_finder = LRFinder(
    new_model, new_optimizer, multi_loss_fn, device=device
)
lr_finder.range_test(train_loader, end_lr=1e-1, num_iter=100)
lr_finder.plot(log_lr=True)
lr_finder.reset()
```



Not quite a "U" shape, but we still can tell that something in the ballpark of 1e-2 is a good starting point.

# **Adaptive Learning Rate**

That's what the **Adam** optimizer is actually doing for us—it starts with the learning rate provided as an argument, but it **adapts** the learning rate(s) as it goes, tweaking it in a different way for each parameter in the model. Or **does it**?

Truth to be told, Adam does not adapt the learning rate—it really adapts the gradients. But, since the parameter update is given by the multiplication of both terms, the learning rate and the gradient, this is a distinction without a difference.

Adam combines the characteristics of two other optimizers: SGD (with momentum) and RMSProp. Like the former, it uses a **moving average of gradients** instead of gradients themselves (that's the *first moment*, in statistics jargon); like the latter, it scales the gradients using a **moving average of squared gradients** (that's the *second moment*, or uncentered variance, in statistics jargon).

But this is not a simple average. It is a **moving average**. And it is not *any* moving average. It is an **exponentially weighted moving average** (EWMA).

Before diving into EWMAs, though, we need to briefly go over simple moving averages.

## **Moving Average (MA)**

To compute the moving average of a given feature x over a certain number of *periods*, we just have to average the values observed over that many time steps (from an initial value observed *periods-1* steps ago all the way up to the *current value*):

$$MA_t(periods, x) = \frac{1}{periods}(x_t + x_{t-1} + \dots + x_{t-periods+1})$$

Equation 6.1 - Simple moving average

But, instead of averaging the values themselves, let's compute the average age of the values. The current value has an age equals one unit of time while the oldest

**value** in our moving average has an **age equals** *periods* units of time, so the **average age** is given by the formula below:

average 
$$age_{MA} = \frac{1 + 2 + \dots + periods}{periods} = \frac{periods + 1}{2}$$

Equation 6.2 - Average age of a moving average

For a **five-period moving average**, the **average age** of its values is **three** units of time.



"Why do we care about the average age of the values?"

This may seem a bit silly in the context of a simple moving average, sure. But, as you'll see in the next sub-section, an **EWMA does not use the number of periods directly** in its formula: We'll have to rely on the **average age** of its values to estimate its (equivalent) number of periods.



"Why use an EWMA then?"

## **EWMA**

An EWMA is more **practical** to compute than a traditional moving average because it **has only two inputs**: The value of **EWMA in the previous step** and the **current value** of the variable being averaged. There are two ways of representing its formula, using alpha or beta:

$$EWMA_{t}(\alpha, x) = \alpha x_{t} + (1 - \alpha)EWMA_{t-1}(\alpha, x)$$

$$EWMA_{t}(\beta, x) = (1 - \beta)x_{t} + \beta EWMA_{t-1}(\beta, x)$$
Equation 6.3 - EWMA

The first alternative, using alpha as the weight of the current value, is most common in other fields, like finance. But, for some reason, the beta alternative is the one commonly found when the Adam optimizer is discussed.

Let's take the first alternative and **expand the equation** a bit:

$$\begin{aligned}
\text{EWMA}_{t}(\alpha, x) &= & \alpha x_{t} &+ (1 - \alpha) (\alpha x_{t-1} &+ (1 - \alpha) \text{ EWMA}_{t-2}(\alpha, x)) \\
&= & \alpha x_{t} &+ (1 - \alpha) \alpha x_{t-1} &+ (1 - \alpha)^{2} \alpha x_{t-2} + \dots \\
&= & (1 - \alpha)^{0} \alpha x_{t-0} &+ (1 - \alpha)^{1} \alpha x_{t-1} &+ (1 - \alpha)^{2} \alpha x_{t-2} + \dots \\
&= \alpha & ((1 - \alpha)^{0} x_{t-0} &+ (1 - \alpha)^{1} x_{t-1} &+ (1 - \alpha)^{2} x_{t-2} + \dots)
\end{aligned}$$

Equation 6.4 - EWMA - expanded edition

The first element is taken at face value, but all the remaining elements are discounted based on their corresponding lags.



"What is a lag?"

It is simply the **distance**, **in units of time**, **from the current value**. So, the value of feature *x* **one time unit in the past** is the value of feature *x* **at lag one**.

After working out the expression above, we end up with an expression where each term has an **exponent** depending on the corresponding **number of lags**. We can use this information to make a sum out of it:

$$EWMA_t(\alpha, x) = \alpha \sum_{\text{lag}=0}^{T-1} \underbrace{(1-\alpha)^{\text{lag}}}_{\text{weight}} x_{t-\text{lag}}$$

Equation 6.5 - EWMA - lag-based

In the expression above, **T** is the **total number of observed values**. So, an EWMA **takes every value into account**, no matter how far in the past it is. But, due to the **weight** (the discount factor), the **older** a value gets, the **less it contributes** to the sum.



Higher values of alpha correspond to rapidly shrinking weights; that is, older values barely make a difference.

Let's see how the **weights** are distributed over the lags for two averages, an EWMA with alpha equals one-third and a simple five-period moving average.

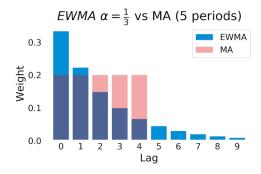


Figure 6.15 - Distribution of weights over lags

See the difference? In a simple **moving average** every value has the **same weight**; that is, they contribute equally to the average. But, in an **EWMA**, more **recent** values have **larger weights** than older ones.

It may not seem like it, but the **two averages** above have **something in common**. The **average age** of their values is approximately the same. Cool, right?

So, if the average age of the values in a five-period moving average is three, we should arrive at (approximately) the same value for the age of the values in the EWMA above. Let's understand why this is so. Maybe you haven't noticed it yet, but a lag of zero corresponds to an age of one unit of time, a lag of one corresponds to an age of two units of time, and so on. We can use this information to compute the average age of the values in an EWMA:

average age<sub>EWMA</sub> = 
$$\alpha \sum_{\text{lag}=0}^{T-1} (1 - \alpha)^{\text{lag}} (\text{lag} + 1) \approx \frac{1}{\alpha}$$

Equation 6.6 - Average age of an EWMA

As the total number of observed values (*T*) grows, the **average age** approaches the **inverse of alpha**. No, I am not demonstrating this here. Yes, I am showing you a snippet of code that "*proves*" it numerically:-)

You may go bananas with the value of **T** trying in vain to approach infinity, but 20 periods is more than enough to make a point:

```
alpha = 1/3; T = 20
t = np.arange(1, T + 1)
age = alpha * sum((1 - alpha)**(t - 1) * t)
age
```

## Output

```
2.9930832408241015
```

That's **three-ish** enough, right? If you're not convinced, try using 93 periods (or more).

Now that we know how to compute the **average age** of an EWMA **given its alpha**, we can figure out **which (simple) moving average** has the **same average age**:

average age = 
$$\frac{\text{periods} + 1}{2} = \frac{1}{\alpha} \implies \alpha = \frac{2}{\text{periods} + 1}$$
;  $\text{periods} = \frac{2}{\alpha} - 1$ 

Equation 6.7 - Alpha vs. periods

There we go, an easy and straightforward relationship between the **value of alpha** and the **number of periods** of a moving average. Guess what happens if you plug the value **one-third** for alpha? You get the corresponding number of periods: **five**. An EWMA using an alpha equal to one-third corresponds to a five-period moving average.

It also works the other way around: If we'd like to compute the EWMA equivalent to a 19-period moving average, the corresponding alpha would be 0.1. And, if we're using the EWMA's formula based on beta, that would be 0.9. Similarly, to compute the EWMA equivalent to a 1999-period moving average, alpha and beta would be 0.001 and 0.999, respectively.

These choices are **not random** at all: It turns out, **Adam** uses these **two values** for its **betas** (one for the moving average of gradients, the other for the moving average of squared gradients).

In code, the implementation of the alpha version of EWMA looks like this:

```
def EWMA(past_value, current_value, alpha):
    return (1- alpha) * past_value + alpha * current_value
```

For computing it over a series of values, given a period, we can define a function like this:

```
def calc_ewma(values, period):
    alpha = 2 / (period + 1)
    result = []
    for v in values:
        try:
            prev_value = result[-1]
        except IndexError:
            prev_value = 0

        new_value = EWMA(prev_value, v, alpha)
        result.append(new_value)
    return np.array(result)
```

In the try..except block, you can see that, if there is no previous value for the EWMA (as in the very first step), it assumes a previous value of zero.

The way the EWMA is constructed has its issues—since it does not need to keep track of all the values inside its period, in its **first steps**, the "average" will be **way off** (or *biased*). For an alpha=0.1 (corresponding to the 19-periods average), the very first "average" will be exactly the first value divided by ten.

To address this issue, we can compute the bias-corrected EWMA:

Bias Corrected EWMA<sub>t</sub>
$$(x, \beta) = \frac{1}{1 - \beta^t}$$
EWMA<sub>t</sub> $(x, \beta)$ 

Equation 6.8 - Bias-corrected EWMA

The beta in the formula above is the same as before: 1 - alpha. In code, we can implement the correction factor like this:

```
def correction(averaged_value, beta, steps):
    return averaged_value / (1 - (beta ** steps))
```

For computing the corrected EWMA over a series of values, we can use a function like this:

```
def calc_corrected_ewma(values, period):
    ewma = calc_ewma(values, period)

alpha = 2 / (period + 1)
    beta = 1 - alpha

result = []
    for step, v in enumerate(ewma):
        adj_value = correction(v, beta, step + 1)
        result.append(adj_value)

return np.array(result)
```

Let's apply both EWMAs, together with a *regular* moving average, to a sequence of **temperature values** to illustrate the differences:

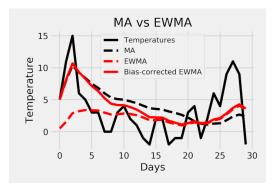


Figure 6.16 - Moving average vs EWMA

As expected, the EWMA without correction (red dashed line) is way off at the beginning, while the regular moving average (black dashed line) tracks the actual values much closer. The **corrected EWMA**, though, does a very good job tracking the actual values from the very beginning. Sure enough, after 19 days, the two EWMAs are barely distinguishable.

## **EWMA Meets Gradients**

Who cares about temperatures, anyway? Let's apply the EWMAs to our gradients, Adam-style!

For each parameter, we compute two EWMAs: one for its gradients, the other for the square of its gradients. Next, we use both values to compute the adapted gradient for that parameter:

$$adapted gradient_t = \frac{Bias Corrected EWMA_t(\beta_1, gradients)}{\sqrt{Bias Corrected EWMA_t(\beta_2, gradients^2)} + \epsilon}$$

Equation 6.9 - Adapted gradient

There they are: Adam's beta1 and beta2 parameters! Its default values, 0.9 and 0.999, correspond to averages of 19 and 1999 periods, respectively.

So, it is a **short-term** average for **smoothing the gradients**, and a **very long-term** average for **scaling the gradients**. The **epsilon** value in the denominator (usually 1e-8) is there only to prevent numerical issues.

Once the adapted gradient is computed, it replaces the actual gradient in the parameter update:

$$SGD: param_t = param_{t-1} - \eta gradient_t$$

Adam: 
$$param_t = param_{t-1} - \eta$$
 adapted gradient<sub>t</sub>

Equation 6.10 - Parameter update

Clearly, the **learning rate** (the Greek letter *eta*) is left untouched!

Moreover, as a result of the **scaling**, the **adapted gradient** is likely to be inside the [-3, 3] range most of the time (this is akin to the standardization procedure but without subtracting the mean).

#### Adam

So, choosing the **Adam** optimizer is an easy and straightforward way to tackle your learning rate needs. Let's take a closer look at PyTorch's <u>Adam</u> optimizer and its arguments:

- params: model's parameters
- 1r: learning rate, default value 1e-3
- betas: tuple containing beta1 and beta2 for the EWMAs
- eps: the epsilon (1e-8) value in the denominator

The four arguments above should be clear by now. But there are two others we haven't talked about yet:

- weight\_decay: L2 penalty
- amsgrad: if the AMSGrad variant should be used

The first argument, weight decay, introduces a regularization term (L2 penalty) to the model's weights. As with every regularization procedure, it aims to prevent overfitting by penalizing weights with large values. The term weight decay comes from the fact that the regularization actually increases the gradients by adding the weight value multiplied by the weight decay argument.



"If it increases the gradients, how come it is called weight decay?"

In the **parameter update**, the gradient is multiplied by the learning rate and **subtracted from the weight's previous value**. So, in effect, adding a penalty to the value of the gradients makes the weights smaller. The smaller the weights, the smaller the penalty, thus making further reductions even smaller—in other words, the weights are decaying.

The second argument, amsgrad, makes the optimizer compatible with a variant of the same name. In a nutshell, it modifies the formula used to compute *adapted gradients*, ditching the bias correction and using the peak value of the EWMA of squared gradients instead.

For now, we're sticking with the first four, well-known to us, arguments:

## **Visualizing Adapted Gradients**

Now, I'd like to give you the chance to **visualize** the gradients, the EWMAs, and the resulting **adapted gradients**. To make it easier, let's bring back our **simple linear regression** problem from *Part I* of this book and, somewhat nostalgically, **perform the training loop** so that we can **log the gradients**.



From now on and until the end of the "Learning Rates" section, we'll be ONLY using the **simple linear regression** dataset to illustrate the effects of different parameters on the minimization of the loss. We'll get back to the *Rock Paper Scissors* dataset in the "Putting It All Together" section.

First, we generate the data points again and run the typical data preparation step (building dataset, splitting it, and building data loaders):

Data Generation & Preparation

```
%run -i data_generation/simple_linear_regression.py
%run -i data_preparation/v2.py
```

Then, we go over the model configuration and change the optimizer from SGD to Adam:

Model Configuration

```
1 torch.manual_seed(42)
2 model = nn.Sequential()
3 model.add_module('linear', nn.Linear(1, 1))
4 optimizer = optim.Adam(model.parameters(), lr=0.1)
5 loss_fn = nn.MSELoss(reduction='mean')
```

We would be ready to use the StepByStep class to *train* our model if it weren't for a minor detail: We still do not have a way of **logging gradients**. So, let's tackle this issue by adding yet another method to our class: capture\_gradients(). Like the attach\_hooks() method, it will take a list of layers that should be monitored for

their gradient values.

For each monitored layer, it will go over its parameters, and, for those that *require* gradients, it will **create a logging function (log\_fn())** and **register a hook** for it in the **tensor corresponding to the parameter**.

The logging function simply appends the gradients to a list in the dictionary entry corresponding to the layer and parameter names. The dictionary itself, \_gradients, is an attribute of the class (which will be created inside the constructor method, but we're setting it manually using setattr for now). The code looks like this:

## StepByStep Method

```
setattr(StepByStep, '_gradients', {})
def capture_gradients(self, layers_to_hook):
    if not isinstance(layers_to_hook, list):
        layers_to_hook = [layers_to_hook]
    modules = list(self.model.named_modules())
    self._gradients = {}
    def make_log_fn(name, parm_id):
        def log_fn(grad):
            self._gradients[name][parm_id].append(grad.tolist())
            return None
        return log_fn
    for name, layer in self.model.named modules():
        if name in layers to hook:
            self._gradients.update({name: {}})
            for parm_id, p in layer.named_parameters():
                if p.requires_grad:
                    self._gradients[name].update({parm_id: []})
                    log_fn = make_log_fn(name, parm_id)
                    self.handles[f'{name}.{parm id}.grad'] = \
                        p.register_hook(log_fn)
    return
setattr(StepByStep, 'capture_gradients', capture_gradients)
```

**IMPORTANT**: The logging function **must return None**, otherwise **the gradients will be modified**, assuming the **returned value**.



The <u>register hook()</u> method registers a **backward hook** to a **tensor for a given parameter**. The **hook function** takes a **gradient as input** and returns either a **modified gradient** or **None**. The hook function will be called every time a gradient with respect to that tensor is computed.

Since we're using this function for *logging purposes*, we should leave the gradients alone and return **None**.



"Isn't there a register\_backward\_hook() method? Why aren't we using it?"

That's a fair question. At the time of writing, this method still has an unsolved issue, so we're following the recommendation of using register\_hook() for individual tensors instead.

Now, we can use the new method to *log gradients* for the linear layer of our model, never forgetting to **remove the hooks** after training:

## **Model Training**

```
1 sbs_adam = StepByStep(model, loss_fn, optimizer)
2 sbs_adam.set_loaders(train_loader)
3 sbs_adam.capture_gradients('linear')
4 sbs_adam.train(10)
5 sbs_adam.remove_hooks()
```

By the time training is finished, we'll have collected two series of 50 gradients each (each epoch has *five mini-batches*), each series corresponding to a parameter of linear (weight and bias), both of them stored in the \_gradients attribute of our StepByStep instance.

We can use these values to compute the EWMAs and the adapted gradients actually used by Adam to update the parameters. Let's do it for the weight parameter:

```
gradients = np.array(
   sbs_adam._gradients['linear']['weight']
).squeeze()

corrected_gradients = calc_corrected_ewma(gradients, 19)
corrected_sq_gradients = calc_corrected_ewma(
   np.power(gradients, 2), 1999
)
adapted_gradients = (corrected_gradients /
   (np.sqrt(corrected_sq_gradients) + 1e-8))
```

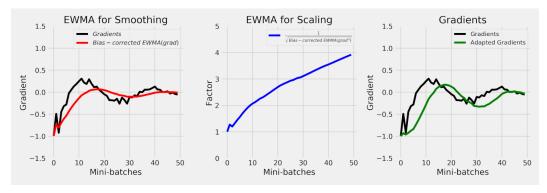


Figure 6.17 - Computing adapted gradients using EWMAs

On the left plot, we see that the bias-corrected EWMA of gradients (in red) is smoothing the gradients. In the center, the bias-corrected EWMA of squared gradients is used for scaling the smoothed gradients. On the right, both EWMAs are combined to compute the adapted gradients.

Under the hood, Adam keeps two values for each parameter, exp\_avg and exp\_avg\_sq, representing the (uncorrected) EWMAs for gradients and squared gradients, respectively. We can take a peek at this using the optimizer's state\_dict():

```
optimizer.state_dict()
```

```
{'state': {140601337662512: {'step': 50,
    'exp_avg': tensor([[-0.0089]], device='cuda:0'),
    'exp_avg_sq': tensor([[0.0032]], device='cuda:0')},
140601337661632: {'step': 50,
    'exp_avg': tensor([0.0295], device='cuda:0'),
    'exp_avg_sq': tensor([0.0096], device='cuda:0')}},
'param_groups': [{'lr': 0.1,
    'betas': (0.9, 0.999),
    'eps': 1e-08,
    'weight_decay': 0,
    'amsgrad': False,
    'params': [140601337662512, 140601337661632]}
```

Inside the dictionary's state key, it contains two other dictionaries (with weird numeric keys) representing the different parameters of the model. In our example, the first dictionary (140614347109072) corresponds to the weight parameter. Since we've logged all the gradients, we should be able to use our calc\_ewma() function to replicate the values contained in the dictionary:

```
(calc_ewma(gradients, 19)[-1],
calc_ewma(np.power(gradients, 2), 1999)[-1])
```

#### Output

```
(-0.008938403644834258, 0.0031747136253540394)
```

Taking the **last values** of our two uncorrected EWMAs, we **matched** the state of the optimizer (exp\_avg and exp\_avg\_sq). Cool!



"OK, cool, but how is it better than SGD in practice?"

Fair enough! We've been discussing how different the parameter update is, but now it is time to show how it affects model training. Let's bring back the loss surface we've computed for this linear regression (way back in Chapter 0) and visualize the path taken by each optimizer to bring both parameters (closer) to their optimal values. That would be great, but we're missing another minor detail: We also do not have a way of logging the evolution of parameters. Guess what

we're gonna do about that? Create another method, of course!

The new method, aptly named capture\_parameters(), works in a way similar to capture\_gradients(). It keeps a dictionary (parameters) as an attribute of the class and **registers forward hooks** to the layers we'd like to log the parameters for. The logging function simply loops over the parameters of a given layer and appends their values to the corresponding entry in the dictionary. The registering itself is handled by a method we developed earlier: attach\_hooks(). The code looks like this:

## StepByStep Method

```
setattr(StepByStep, '_parameters', {})
def capture_parameters(self, layers_to_hook):
    if not isinstance(layers_to_hook, list):
        layers_to_hook = [layers_to_hook]
    modules = list(self.model.named modules())
    layer_names = {layer: name for name, layer in modules}
    self._parameters = {}
    for name, layer in modules:
        if name in layers to hook:
            self._parameters.update({name: {}})
            for parm_id, p in layer.named_parameters():
                self._parameters[name].update({parm_id: []})
    def fw_hook_fn(layer, inputs, outputs):
        name = layer_names[layer]
        for parm_id, parameter in layer.named_parameters():
            self._parameters[name][parm_id].append(
                parameter.tolist()
            )
    self.attach_hooks(layers_to_hook, fw_hook_fn)
    return
setattr(StepByStep, 'capture_parameters', capture_parameters)
```

What's next? We need to create two instances of StepByStep, each using a

different optimizer, set them to capture parameters, and train them for ten epochs. The captured parameters (bias and weight) will draw the following paths (the red dot represents their optimal values).

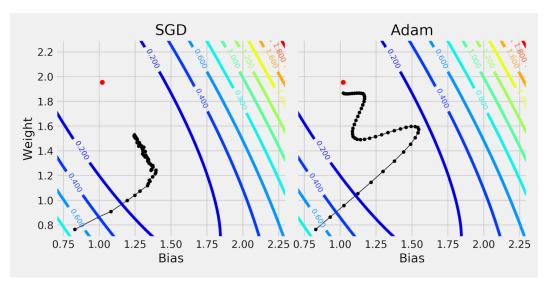


Figure 6.18 - Paths taken by SGD and Adam

On the left plot, we have the typical well-behaved (and slow) path taken by **simple gradient descent**. You can see it is **wiggling** a bit due to the noise introduced by using **mini-batches**. On the right plot, we see the effect of using the exponentially weighted moving averages: On the one hand, **it is smoother and moves faster**; on the other hand, it **overshoots** and has to **change course back and forth** as it approaches the target. It is **adapting to the loss surface**, if you will.



If you like the idea of visualizing (and animating) the paths of optimizers, make sure to check out <u>Louis Tiao's tutorial</u> on the subject.

Talking about losses, we can also compare the trajectories of training and validation losses for each optimizer.



Figure 6.19 - Losses (SGD and Adam)

Remember, the losses are computed at the end of each epoch by averaging the losses of the mini-batches. On the left plot, even if SGD wiggles a bit, we can see that every epoch shows a lower loss than the previous one. On the right plot, the **overshooting** becomes clearly visible as an **increase in the training loss**. But it is also clear that Adam achieves a **lower loss** because it got **closer to the optimal value** (the red dot in the previous plot).



In real problems, where it is virtually **impossible to plot the loss surface**, we can look at the **losses** as an "*executive summary*" of what's going on. Training losses will sometimes go up before they go down again, and this is expected.

# **Stochastic Gradient Descent (SGD)**

Adaptive learning rates are cool, indeed, but good old stochastic gradient descent (SGD) also has a couple of tricks up its sleeve. Let's take a closer look at PyTorch's <u>SGD</u> optimizer and its arguments:

- params: model's parameters
- 1r: learning rate
- weight\_decay: L2 penalty

The three arguments above are already known. But there are three new arguments:

• momentum: momentum factor, SGD's own beta argument, is the topic of the next section

- dampening: dampening factor for momentum
- nesterov: enables Nesterov momentum, which is a smarter version of the regular momentum, and also has its own section

That's the perfect moment to dive deeper into momentum (sorry, I really cannot miss a pun!).

#### **Momentum**

One of SGD's tricks is called **momentum**. At first sight, it looks very much like using an EWMA for gradients, but it isn't. Let's compare EWMA's beta formulation with momentum's:

$$EWMA_{t} = (1 - \beta) \operatorname{grad}_{t} + \beta EWMA_{t-1}$$

$$momentum_{t} = \operatorname{grad}_{t} + \beta \operatorname{momentum}_{t-1}$$

Equation 6.11 - Momentum vs EWMA

See the difference? It does not average the gradients; it runs a cumulative sum of "discounted" gradients. In other words, all past gradients contribute to the sum, but they are "discounted" more and more as they grow older. The "discount" is driven by the beta parameter. We can also write the formula for momentum like this:

$$\mathrm{momentum}_t = \beta^0 \ \mathrm{grad}_t + \beta^1 \ \mathrm{grad}_{t-1} + \beta^2 \ \mathrm{grad}_{t-2} + \ldots + \beta^n \ \mathrm{grad}_{t-n}$$
 Equation 6.12 - Compounding momentum

The disadvantage of this second formula is that it requires the *full history* of gradients, while the previous one depends only on the gradient's current value and momentum's latest value.



"What about the dampening factor?"

The dampening factor is a way to, well, dampen the effect of the latest gradient. Instead of having its full value added, the latest gradient gets its contribution to momentum reduced by the dampening factor. So, if the dampening factor is 0.3, only 70% of the latest gradient gets added to momentum. Its formula is given by:

$$momentum_t = (1 - damp) \operatorname{grad}_t + \beta \operatorname{momentum}_{t-1}$$

Equation 6.13 - Momentum with dampening factor



If the dampening factor equals the momentum factor (beta), it becomes a true EWMA!

Similar to Adam, SGD with momentum keeps the value of momentum for each parameter. The beta parameter is stored there as well (momentum). We can take a peek at it using the optimizer's state\_dict():

```
{'state': {139863047119488: {'momentum_buffer': tensor([[-
0.0053]])},
    139863047119168: {'momentum_buffer': tensor([-0.1568])}},
    'param_groups': [{'lr': 0.1,
        'momentum': 0.9,
        'dampening': 0,
        'weight_decay': 0,
        'nesterov': False,
        'params': [139863047119488, 139863047119168]}]}
```

Even though old gradients slowly fade away, contributing less and less to the sum, very recent gradients are taken almost at their face value (assuming a typical value of 0.9 for beta and no dampening). This means that, given a sequence of all positive (or all negative) gradients, their sum, that is, the momentum, is going up really fast (in absolute value). A large momentum gets translated into a large update since momentum replaces gradients in the parameter update:

```
\begin{aligned} \text{SGD}: \ \operatorname{param}_t &= \operatorname{param}_{t-1} - \eta \ \operatorname{gradient}_t \\ \operatorname{Adam}: \ \operatorname{param}_t &= \operatorname{param}_{t-1} - \eta \ \operatorname{adapted} \ \operatorname{gradient}_t \\ \operatorname{SGD} \ \operatorname{with} \ \operatorname{Momentum}: \ \operatorname{param}_t &= \operatorname{param}_{t-1} - \eta \ \operatorname{momentum}_t \\ &= \operatorname{Equation} \textit{6.14-Parameter update} \end{aligned}
```

This behavior can be easily visualized in the path taken by SGD with momentum.

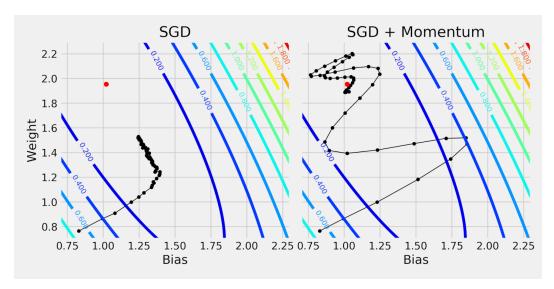


Figure 6.20 - Paths taken by SGD (with and without momentum)

Like the Adam optimizer, SGD with momentum **moves faster** and **overshoots**. But it does seem to get **carried away** with it, so much so that it **gets past the target** and has to **backtrack** to approach it from a different direction.

The analogy for the momentum update is that of a **ball rolling down a hill**: It picks up so much speed that it ends up climbing the opposite side of the valley, only to roll back down again with a little bit less speed, doing this back and forth over and over again until eventually reaching the bottom.



"Isn't Adam better than this already?"

Yes and no. Adam indeed converges more quickly to *a* minimum, but not necessarily a *good* one. In a simple linear regression, there is a **global minimum** corresponding to the **optimal value of the parameters**. This is **not the case in deep learning models**: There are **many minima** (plural of minimum), and **some are better than others** (corresponding to lower losses). So, Adam will find one of these minima and move there fast, perhaps overlooking better alternatives in the neighborhood.

Momentum may seem a bit *sloppy* at first, but it may be **combined with a learning rate scheduler** (more on that shortly!) to **better explore the loss surface** in hopes of finding a better-quality minimum than Adam does.



Both alternatives, **Adam** and **SGD with momentum** (especially when combined with a learning rate scheduler), are commonly used.

But, if a ball running downhill seems a bit too out of control for your taste, maybe you'll like its variant better...

#### Nesterov

The Nesterov accelerated gradient (NAG), or Nesterov for short, is a clever variant of SGD with momentum. Let's say we're computing **momentum** for two consecutive steps (t and t+1):

step t : 
$$\mathbf{mo}_t = \operatorname{grad}_t + \beta \ \mathbf{mo}_{t-1}$$
 step t+1 :  $\mathbf{mo}_{t+1} = \operatorname{grad}_{t+1} + \beta \ \mathbf{mo}_t$ 

Equation 6.15 - Nesterov momentum

In the current step (t), we use the current gradient (t) and the momentum from the previous step (t-1) to compute the current momentum. So far, nothing new.

In the next step (t+1), we'll use the next gradient (t+1) and the momentum we've just computed for the current step (t) to compute the next momentum. Again, nothing new.

What if I ask you to compute momentum one step ahead?



"Can you tell me momentum at step t+1 while you're still at step t?"

"Of course I can't, I do not know the **gradient at step t+1**!" you say, puzzled at my bizarre question. Fair enough. So I ask you yet another question:



"What's your best guess for the gradient at step t+1?"

I hope you answered, "The gradient at step t." If you do not know the future value of a variable, the naive estimate is its current value. So, let's go with it, Nesterov-style!

In a nutshell, what NAG does is **try to compute momentum one step ahead** since it is only missing one value and has a good (naive) guess for it. It is as if it were computing momentum **between two steps**:

$$\begin{aligned} &\text{step t:} &&\text{mo}_t = & \text{grad}_t + \beta & \text{mo}_{t-1} \\ &\text{step t:} & \text{nesterov}_t = & \text{grad}_t + \beta & \text{mo}_t \\ &\text{step t+1:} && \text{mo}_{t+1} = & \text{grad}_{t+1} + \beta & \text{mo}_t \end{aligned}$$

Once Nesterov's momentum is computed, it **replaces the gradient in the parameter update**, just like regular momentum does:

Equation 6.16 - Looking ahead

SGD with Momentum : 
$$param_t = param_{t-1} - \eta mo_t$$
  
SGD with Nesterov :  $param_t = param_{t-1} - \eta nesterov_t$ 

Equation 6.17 - Parameter update

But, Nesterov actually uses momentum, so we can expand its expression like this:

$$\begin{aligned} \text{param}_t &= \text{param}_{t-1} - \eta \text{ nesterov}_t \\ &= \text{param}_{t-1} - \eta \text{ (grad}_t + \beta \text{ mo}_t) \\ &= \text{param}_{t-1} - \eta \text{ grad}_t - \beta \eta \text{ mo}_t \end{aligned}$$

Equation 6.18 - Parameter update (expanded)



"Why did you do this? What's the purpose of making the formula more complicated?"

You'll understand why in a minute :-)

#### Flavors of SGD

Let's compare the three flavors of SGD, vanilla (regular), momentum, and Nesterov, when it comes to the way they perform the **parameter update**:

$$\begin{aligned} & \text{SGD}: \ \text{param}_t = \text{param}_{t-1} \ - \eta \ \text{grad}_t \\ & \text{SGD with Momentum}: \ \text{param}_t = \text{param}_{t-1} \ - \eta \ \text{mo}_t \\ & \text{SGD with Nesterov}: \ \text{param}_t = \text{param}_{t-1} \ - \eta \ \text{grad}_t \ - \beta \ \eta \ \text{mo}_t \\ & & \text{Equation 6.19-Flavors of parameter update} \end{aligned}$$

That's why I expanded Nesterov's expression in the last section: It is easier to compare the updates this way! First, there is **regular SGD**, which uses the **gradient and nothing else**. Then, there is **momentum**, which uses a "*discounted*" sum of past

**gradients** (the momentum). Finally, there is **Nesterov**, which **combines both** (with a small tweak).

How different are the updates? Let's check it out! The plots below show the **update term** (before multiplying it by the learning rate) for the **weight** parameter of our linear regression.

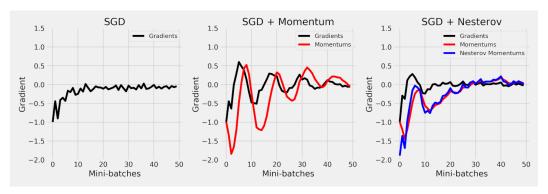


Figure 6.21 - Update terms corresponding to SGD flavors

Does the **shape of the update term for SGD with momentum** ring a bell? The oscillating pattern was already depicted in the **path taken by SGD with momentum** while optimizing the two parameters: When it **overshoots**, it has to **reverse direction**, and by repeatedly doing that, these oscillations are produced.

Nesterov momentum seems to do a better job: The **look-ahead** has the effect of **dampening the oscillations** (please do not confuse this effect with the actual *dampening* argument). Sure, the idea *is* to look ahead to avoid going too far, but could you have told me the difference between the two plots beforehand? Me neither! Well, I am *assuming* you replied "no" to this question, and that's why I thought it was a good idea to illustrate the patterns above.



"How come the black lines are different in these plots? Isn't the **underlying gradient** supposed to be the same?"

The gradient is indeed *computed the same way* in all three flavors, but since the **update terms are different**, the gradients are **computed at different locations of the loss surface**. This becomes clear when we look at the paths taken by each of the flavors.

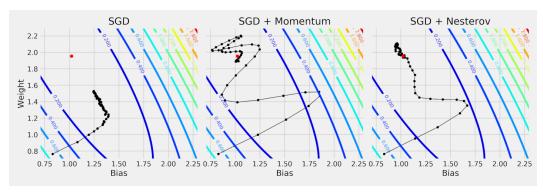


Figure 6.22 - Path taken by each SGD flavor

Take the *third point* in the lower-left part of the black line, for instance: Its location is quite different in each of the plots and thus so are the corresponding gradients.

The two plots on the left are already known to us. The new plot in town is the one to the right. The **dampening of the oscillations** is abundantly clear, but Nesterov's momentum **still gets past its target** and has to **backtrack** a little to approach it from the opposite direction. And let me remind you that this is **one of the easiest loss surfaces of all!** 

Talking about losses, let's take a peek at their trajectories.



Figure 6.23 - Losses for each SGD flavor

The plot on the left is there just for comparison; it is the same as before. The one on the right is quite straightforward too, depicting the fact that Nesterov's momentum quickly found its way to a lower loss and slowly approached the optimal value.

The plot in the middle is a bit more intriguing: Even though **regular momentum** produced a path with **wild swings** over the loss surface (each black dot corresponds to a mini-batch), its **loss trajectory** oscillates less than Adam's does. This is an artifact of this simple linear regression problem (namely, the bowl-shaped loss surface), and should not be taken as representative of typical behavior.

If you're not convinced by *momentum*, either regular or Nesterov, let's add something else to the mix...

# **Learning Rate Schedulers**

It is also possible to **schedule** the changes in the **learning rate** as training goes, instead of adapting the gradients. Say you'd like to **reduce the learning rate by one order of magnitude** (that is, multiplying it by 0.1) **every** *T* **epochs**, such that training is **faster at the beginning** and **slows down** after a while to try avoiding convergence problems.



That's what a **learning rate scheduler** does: It **updates the learning rate of the optimizer**.

So, it should be no surprise that one of the scheduler's arguments is the optimizer itself. The learning rate set for the optimizer will be the initial learning rate of the scheduler. As an example, let's take the simplest of the schedulers: StepLR, which simply multiplies the learning rate by a factor gamma every step\_size epochs.

In the code below, we create a dummy optimizer, which is "updating" some fake parameter with an initial learning rate of 0.01. The dummy scheduler, an instance of StepLR, will multiply that learning rate by 0.1 every two epochs.

```
dummy_optimizer = optim.SGD([nn.Parameter(torch.randn(1))], lr=0.01)
dummy_scheduler = StepLR(dummy_optimizer, step_size=2, gamma=0.1)
```

The **scheduler** has a **step()** method just like the optimizer.



You should call the scheduler's step() method after calling the optimizer's step() method.

Inside the training loop, it will look like this:

```
for epoch in range(4):
    # training loop code goes here

    print(dummy_scheduler.get_last_lr())
    # First call optimizer's step
    dummy_optimizer.step()
    # Then call scheduler's step
    dummy_scheduler.step()

dummy_optimizer.zero_grad()
```

#### Output

```
[0.01]
[0.01]
[0.001]
[0.001]
```

As expected, it kept the initial learning rate for two epochs and then multiplied it by 0.1, resulting in a learning rate of 0.001 for another two epochs. In a nutshell, that's how a learning rate scheduler works.



"Does every scheduler **shrink** the learning rate?"

Not really, no. It used to be standard procedure to *shrink* the learning rate as you train the model, but this idea was then challenged by **cyclical learning rates** (that's the "cyclical" part of Leslie N. Smith's paper!). There are many different flavors of scheduling, as you can see. And many of them are available in PyTorch.

We're dividing schedulers into three groups: schedulers that update the learning rate **every** T **epochs** (even if T=1), like in the example above; the scheduler that only updates the learning rate when the **validation loss seems to be stuck**; and schedulers that update the learning rate after **every mini-batch**.

## **Epoch Schedulers**

These schedulers will have their **step()** method called at the **end of every epoch**. But each scheduler has its own rules for updating the learning rate.

- StepLR: It multiplies the learning rate by a factor gamma every step\_size epochs.
- <u>MultiStepLR</u>: It multiplies the learning rate by a factor gamma at the epochs indicated in the list of milestones.
- **ExponentialLR**: It multiplies the learning rate by a factor gamma every epoch, no exceptions.
- <u>LambdaLR</u>: It takes your own customized function that should take the epoch as an argument and returns the corresponding multiplicative factor (with respect to the <u>initial learning rate</u>).
- <u>CosineAnnealingLR</u>: It uses a technique called cosine annealing to update the learning rate, but we're not delving into details here.

We can use LambdaLR to mimic the behavior of the StepLR scheduler defined above:

```
dummy_optimizer = optim.SGD([nn.Parameter(torch.randn(1))], lr=0.01)
dummy_scheduler = LambdaLR(
    dummy_optimizer, lr_lambda=lambda epoch: 0.1 ** (epoch//2)
)
# The scheduler above is equivalent to this one
# dummy_scheduler = StepLR(dummy_optimizer, step_size=2, gamma=0.1)
```

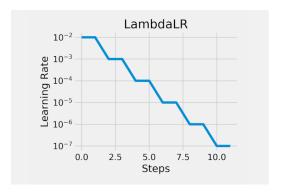


Figure 6.24 - Evolution of learning rate (epoch scheduler)

#### Validation Loss Scheduler

The <u>ReduceLROnPlateau</u> scheduler should <u>also</u> have its step() method called at the end of every epoch, but it has its own group here because it <u>does not follow a predefined schedule</u>. Ironic, right?

The step() method takes the validation loss as an argument, and the scheduler can be configured to tolerate a lack of improvement in the loss (to a threshold, of

course) up to a given number of epochs (the aptly named patience argument). After the scheduler runs out of patience, it updates the learning rate, multiplying it by the factor argument (for the schedulers listed in the last section, this factor was named gamma).

To illustrate its behavior, let's assume the validation loss remains at the same value (whatever that is) for 12 epochs in a row. What would our scheduler do?

```
dummy_optimizer = optim.SGD([nn.Parameter(torch.randn(1))], lr=0.01)
dummy_scheduler = ReduceLROnPlateau(
    dummy_optimizer, patience=4, factor=0.1
)
```



Figure 6.25 - Evolution of learning rate (validation loss scheduler)

Its patience is **four epochs**, so after four epochs observing the same loss, it is hanging by a thread. Then comes the **fifth epoch** with **no change**: "That's it, the learning rate must go down," you can almost hear it saying :-) So, in the **sixth epoch**, the optimizer is already using the newly updated learning rate. If nothing changes for four more epochs, it goes down again, as shown in the figure above.

## Schedulers in StepByStep — Part I

If we want to incorporate learning rate schedulers into our training loop, we need to make some changes to our StepByStep class. Since schedulers are definitely *optional*, we need to add a **method** to allow the user to **set a scheduler** (similar to what we did with TensorBoard integration). Moreover, we need to define some **attributes**: one for the scheduler itself, and a boolean variable to distinguish whether it is an epoch or a mini-batch scheduler.

## StepByStep Method

Next, we create a protected method that invokes the step() method of the scheduler and appends the current learning rate to an attribute, so we can keep track of its evolution.

## StepByStep Method

And then we modify the train() method to include a call to the protected method defined above. It should come after the validation inner loop.

## StepByStep Method

```
def train(self, n_epochs, seed=42):
    # To ensure reproducibility of the training process
    self.set seed(seed)
    for epoch in range(n_epochs):
        # Keeps track of the number of epochs
        # by updating the corresponding attribute
        self.total epochs += 1
        # inner loop
        # Performs training using mini-batches
        loss = self. mini batch(validation=False)
        self.losses.append(loss)
        # VALIDATION
        # no gradients in validation!
        with torch.no_grad():
            # Performs evaluation using mini-batches
            val loss = self. mini batch(validation=True)
            self.val_losses.append(val_loss)
        self. epoch schedulers(val loss) ①
        # If a SummaryWriter has been set...
        if self.writer:
            scalars = {'training': loss}
            if val_loss is not None:
                scalars.update({'validation': val_loss})
            # Records both losses for each epoch under tag "loss"
            self.writer.add_scalars(main_tag='loss',
                                    tag_scalar_dict=scalars,
                                    global_step=epoch)
    if self.writer:
        # Closes the writer
        self.writer.close()
setattr(StepByStep, 'train', train)
```

① Calls the learning rate scheduler at the end of every epoch

#### Mini-Batch Schedulers

These schedulers have their **step() method** called at the **end of every mini-batch**. They are all **cyclical** schedulers.

• <u>CycliclR</u>: This cycles between base\_lr and max\_lr (so it disregards the initial learning rate set in the optimizer), using step\_size\_up updates to go from the base to the max learning rate, and step\_size\_down updates to go back. This behavior corresponds to mode=triangular. Additionally, it is possible to *shrink* the amplitude using different modes: triangular2 will halve the amplitude after each cycle, while exp\_range will exponentially shrink the amplitude using gamma as base and the number of the cycle as the exponent.



A typical choice of value for max\_lr is the learning rate found using the LR Range Test.

- OneCycleLR: This uses a method called annealing to update the learning rate from its initial value up to a defined maximum learning rate (max\_lr) and then down to a much lower learning rate over a total\_steps number of updates, thus performing a single cycle.
- <u>CosineAnnealingWarmRestarts</u>: This uses <u>cosine annealing[103]</u> to update the learning rate, but we're not delving into details here, except to say that this particular scheduler requires the **epoch number** (including the **fractional part** corresponding to the number of mini-batches over the length of the data loader) as an **argument** of its step() method.

Let's try CyclicLR in different modes for a range of learning rates between 1e-4 and 1e-3, two steps in each direction.

```
dummy_parm = [nn.Parameter(torch.randn(1))]
dummy_optimizer = optim.SGD(dummy_parm, lr=0.01)

dummy_scheduler1 = CyclicLR(dummy_optimizer, base_lr=1e-4,
    max_lr=1e-3, step_size_up=2, mode='triangular')
dummy_scheduler2 = CyclicLR(dummy_optimizer, base_lr=1e-4,
    max_lr=1e-3, step_size_up=2, mode='triangular2')
dummy_scheduler3 = CyclicLR(dummy_optimizer, base_lr=1e-4,
    max_lr=1e-3, step_size_up=2, mode='exp_range', gamma=np.sqrt(.5))
```

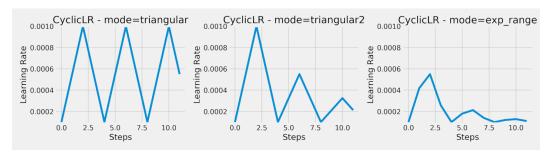


Figure 6.26 - Evolution of learning rate (cyclical scheduler)

By the way, two steps means it would complete a full cycle every four mini-batch updates—that's completely unreasonable, and is only used here to illustrate the behavior.



In practice, a cycle should encompass between **two and ten epochs** (according to Leslie N. Smith's paper), so you need to figure out how many mini-batches your training set contains (that's the **length of the data loader**) and multiply it by the desired number of epochs in a cycle to get the total number of steps in a cycle.

In our example, the train loader has 158 mini-batches, so if we want the learning rate to **cycle over five epochs**, the full cycle should have 790 steps, and thus step\_size\_up should be half that value (395).

## Schedulers in StepByStep — Part II

We need to make some more changes to handle **mini-batch schedulers**. Similar to "Part I" above, we need to create a protected method that handles the step() method of this group of schedulers.

## StepByStep Method

And then we must modify the mini\_batch() method to include a call to the protected method defined above. It should be called at the end of the loop, but only during training.

## StepByStep Method

```
def mini batch(self, validation=False):
    # The mini-batch can be used with both loaders
    # The argument 'validation' defines which loader and
    # corresponding step function are going to be used
    if validation:
        data loader = self.val loader
        step_fn = self.val_step_fn
    else:
        data loader = self.train loader
        step_fn = self.train_step_fn
    if data loader is None:
        return None
    n batches = len(data_loader)
    # Once the data loader and step function are defined;
    # this is the same mini-batch loop we had before
    mini batch losses = []
    for i, (x_batch, y_batch) in enumerate(data_loader):
        x_batch = x_batch.to(self.device)
        y_batch = y_batch.to(self.device)
        mini_batch_loss = step_fn(x_batch, y_batch)
        mini_batch_losses.append(mini_batch_loss)
        if not validation:
            self. mini batch schedulers(i / n batches) ②
    loss = np.mean(mini_batch_losses)
    return loss
setattr(StepByStep, '_mini_batch', _mini_batch)
```

- ① Only during training!
- 2 Calls the learning rate scheduler at the end of every mini-batch update

#### **Scheduler Paths**

Before trying out a couple of schedulers, let's run an LR Range Test on our model:

We're starting really low (lr=1e-3) and testing all the way up to 1.0 (end\_lr) using exponential increments. The results suggest a **learning rate somewhere between 0.01 and 0.1** (corresponding to the center of the descending part of the curve). We know for a fact that a learning rate of 0.1 works. A more conservative choice of value would be 0.025, for instance, since it is a midpoint in the descending part of the curve.

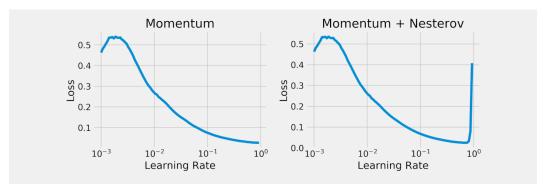


Figure 6.27 - Learning rate finder

Let's be bold! First, we define the optimizer with our choice for initial learning rate (0.1):

```
optimizer = optim.SGD(
    model.parameters(), lr=0.1, momentum=0.9, nesterov=False
)
```

Then, we pick a scheduler to bring the learning rate all the way down to 0.025. If we choose a *step scheduler*, we can cut the learning rate in half (gamma=0.5) every four epochs. If we choose a *cyclical scheduler*, we can oscillate the learning rate between the two extremes every four epochs (20 mini-batches: 10 up, 10 down).

```
step_scheduler = StepLR(optimizer, step_size=4, gamma=0.5)
cyclic_scheduler = CyclicLR(
    optimizer, base_lr=0.025, max_lr=0.1,
    step_size_up=10, mode='triangular2'
)
```

After applying each scheduler to SGD with momentum, and to SGD with Nesterov's momentum, we obtain the following paths:

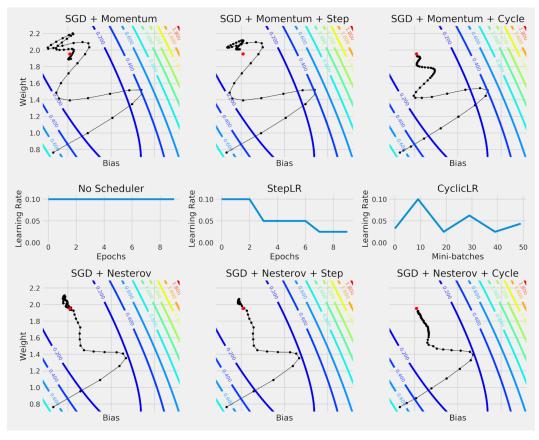


Figure 6.28 - Paths taken by SGD combining momentum and scheduler

Adding a scheduler to the mix seems to have helped the optimizer to achieve a more stable path toward the minimum.



The general idea behind using a scheduler is to allow the optimizer to alternate between **exploring the loss surface** (high learning rate phase) and **targeting a minimum** (low learning rate phase).

What is the impact of the scheduler on loss trajectories? Let's check it out!

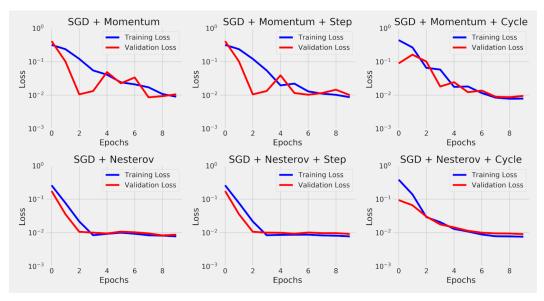


Figure 6.29 - Losses for SGD combining momentum and scheduler

It is definitely harder to tell the difference between curves in the same row, except for the combination of Nesterov's momentum and cyclical scheduler, which produced a smoother reduction in the training loss.

# **Adaptive vs Cycling**

Although adaptive learning rates are considered competitors of cyclical learning rates, this does not prevent you from combining them and cycling learning rates while using Adam. While Adam adapts the gradients using its EWMAs, the cycling policy modifies the learning rate itself, so they can work together indeed.

There is **much more** to learn about in the topic of **learning rates**: This section is meant to be only a short introduction to the topic.

# **Putting It All Together**

In this chapter, we were all over the place: data preparation, model configuration, and model training—a little bit of everything. Starting with a brand-new dataset, *Rock Paper Scissors*, we built a method for **standardizing** the images (for real this time) using a temporary data loader. Next, we developed a fancier model that included **dropout** layers for regularization. Then, we turned our focus to the training part, diving deeper into **learning rates**, **optimizers**, and **schedulers**. We implemented many methods: for finding a learning rate, for capturing gradients and parameters, and for updating the learning rate using a scheduler.

```
1 # Loads temporary dataset to build normalizer
 2 temp transform = Compose([Resize(28), ToImage(),
 3
                             ToDtype(torch.float32, scale=True)])
4 temp dataset = ImageFolder(root='rps', transform=temp transform)
 5 temp_loader = DataLoader(temp_dataset, batch_size=16)
 6 normalizer = StepByStep.make_normalizer(temp_loader)
 7
8 # Builds transformation, datasets, and data loaders
 9 composer = Compose([Resize(28), ToImage(),
10
                       ToDtype(torch.float32, scale=True),
11
                       normalizer])
12 train data = ImageFolder(root='rps', transform=composer)
13 val data = ImageFolder(root='rps-test-set', transform=composer)
14 # Builds a loader of each set
15 train loader = DataLoader(
       train_data, batch_size=16, shuffle=True
16
17)
18 val loader = DataLoader(val data, batch size=16)
```

In the model configuration part, we can use **SGD with Nesterov's momentum** and a **higher dropout probability** to increase regularization:

## **Model Configuration**

Before the actual training, we can run an LR Range Test:

## Learning Rate Range Test

```
1 sbs_cnn3 = StepByStep(model_cnn3, multi_loss_fn, optimizer_cnn3)
2 tracking, fig = sbs_cnn3.lr_range_test(
3 train_loader, end_lr=2e-1, num_iter=100
4 )
```

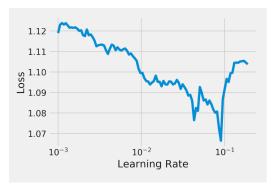


Figure 6.30 - Learning rate finder

The test suggests a learning rate around 0.01, so we recreate the optimizer and set it in our StepByStep instance.

We can also use the suggested learning rate as the **upper range** of a **cyclical scheduler**. For its step size, we can use the length of the data loader, so the learning rate goes all the way up in one epoch, and all the way down in the next—a two-epoch cycle.

## **Updating Learning Rate**

```
1 optimizer_cnn3 = optim.SGD(
2     model_cnn3.parameters(), lr=0.03, momentum=0.9, nesterov=True
3 )
4 sbs_cnn3.set_optimizer(optimizer_cnn3)
5
6 scheduler = CyclicLR(
7     optimizer_cnn3, base_lr=1e-3, max_lr=0.01,
8     step_size_up=len(train_loader), mode='triangular2'
9 )
10 sbs_cnn3.set_lr_scheduler(scheduler)
```

After doing this, it is training as usual:

#### Model Training

```
1 sbs_cnn3.set_loaders(train_loader, val_loader)
2 sbs_cnn3.train(10)
```

```
fig = sbs_cnn3.plot_losses()
```

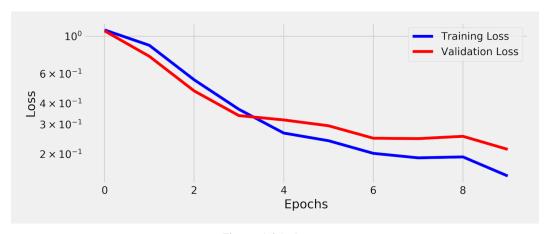


Figure 6.31 - Losses

#### **Evaluation**

## Output

```
tensor([2511, 2520]) tensor([336, 372])
```

Looking good! Lower losses, 99.64% training accuracy, and 90.32% validation accuracy.

# Recap

In this chapter, we've introduced dropout layers for regularization and focused on the inner workings of different optimizers and the role of the learning rate in the process. This is what we've covered:

- computing channel statistics using a temporary data loader to build a Normalize() transform
- using Normalize() to standardize an image dataset
- understanding how convolutions over multiple channels work
- building a fancier model with two typical convolutional blocks and dropout layers

- understanding how the dropout probability generates a distribution of outputs
- observing the **effect of train and eval modes** in dropout layers
- visualizing the regularizing effect of dropout layers
- using the learning rate range test to find an interval of learning rate candidates
- computing bias-corrected exponentially weighted moving averages of both gradients and squared gradients to implement adaptive learning rates like the Adam optimizer
- capturing **gradients** using register\_hook() on tensors of learnable parameters
- capturing parameters using the previously implemented attach\_hooks()
   method
- visualizing the path taken by different optimizers for updating parameters
- understanding how momentum is computed and its effect on the parameter update
- (re)discovering the clever look-ahead trick implemented by Nesterov's momentum
- learning about different types of **schedulers**: epoch, validation loss, and minibatch
- including learning rate schedulers in the training loop
- visualizing the impact of a scheduler on the path taken for updating parameters

Congratulations! You have just learned about the tools commonly used for training deep learning models: adaptive learning rates, momentum, and learning rate schedulers. Far from being an exhaustive lesson on this topic, this chapter has given you a good understanding of the basic building blocks. You have also learned how dropout can be used to reduce overfitting and, consequently, improve generalization.

In the next chapter, we'll learn about **transfer learning** to leverage the power of **pre-trained models**, and we'll go over some key components of popular architectures, like **1x1 convolutions**, **batch normalization** layers, and **residual connections**.

 $[\underline{93}] \underline{https://github.com/dvgodoy/PyTorchStepByStep/blob/master/Chapter06.ipynb}$ 

[94] https://colab.research.google.com/github/dvgodoy/PyTorchStepByStep/blob/master/Chapter06.ipynb

- [95] http://www.samkass.com/theories/RPSSL.html
- [96] https://bit.ly/3F6qp88
- [97] https://storage.googleapis.com/download.tensorflow.org/data/rps.zip
- [98] https://storage.googleapis.com/download.tensorflow.org/data/rps-test-set.zip
- [99] https://twitter.com/karpathy/status/801621764144971776
- [100] https://arxiv.org/abs/1506.01186
- [101] https://pypi.org/project/torch-lr-finder/
- [102] https://tinyurl.com/mvef2sfj
- [103] https://paperswithcode.com/method/cosine-annealing